Umklapp Scattering and Heat Conductivity of Superlattices

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Abstract

The mean free path of phonons in superlattices is estimated. It is shown to be strongly dependent on the superlattice period due to the Umklapp scattering in subbands. It first falls with increasing the superlattice period until it becomes comparable with the latter after what it rises back to the bulk value. Similar behavior is expected of heat conductivity, which is proportional to the mean free path.

Superlattices offer an opportunity to control physical properties in unprecedented ways. Their thermal conductivity is of interest both for a fundamental understanding of these systems as well as in applications. Recently there has been a resurgence of interest in finding materials with improved thermoelectric transport properties for cooling and power generation. The quality of a material for such applications is given by the thermoelectric figure of merit, which is inversely proportional to the thermal conductivity κ. In materials of interest, such as semiconductors, the lattice contribution to κ dominates.

Experimental and theoretical work suggests that the thermal conductivity of superlattices is quite low, both for transport along the planes [1, 2, 10], or perpendicular to the planes [3, 4, 5, 6, 7, 8, 11].

The lattice heat conductivity κ is given approximately by an equation [12]:

$$\kappa \approx Cvl, \tag{1}$$

where C is the lattice heat capacitance, v - the average phonon group velocity, and l - the mean free path. Recently we presented calculations of the thermal conductivity perpendicular to the layers [11] which were done in approximation which takes into account changes in phonon group velocities due to band folding, but neglects the dependence of the phonon mean free path on the superlattice period. The investigation of this dependence is the subject of the present work.

Three-phonon scattering due to anharmonicity is the dominant contribution to the lattice thermal resistivity. Umklapp processes, in which the net phonon momentum change by a reciprocal lattice vector, give the finite thermal conductivity [12]. Only phonons with energies of the order of Debye energy, Θ_D can participate in Umklapp scattering, giving a temperature dependence of the phonon mean free path l of the form [12]

$$l \approx \exp(\Theta_D/T). \tag{2}$$

In superlattices, new mini-bands are introduced in the acoustic phonon dispersions along the growth direction, and they give rise to new Umklapp processes. The lowest phonon energy for Umklapp scattering in a superlattice of period L is of order Θ_D/L and phonon mean free path in a superlattice, L_{sl} becomes:

$$l_{sl} \approx \exp(-\Theta_D/LT). \tag{3}$$

The ratio of the mean free paths is:

$$l_{sl}/l \approx \exp(\Theta_D/T(1/L-1)), \tag{4}$$

which can be rather small for big L and small T.

According to Eq.4 l_{sl} decreases with L and eventually should become $l_{sl} = L$. This shall happen at the value of $L = L_c$ given by a solution to the equation:

$$L_c/l = \exp(\Theta_D/T(1/L_c - 1)) \tag{5}$$

What happens next? When L exceeds L_c according to Eq.4 it should become $l_{sl} < L$. However in this case Eq.4 is no longer applicable because when $l_{sl} < L$ superlattice effects should not matter and l_{sl} should assume the bulk value l. But as $L < l$ then Eq.4 should be valid again. The only resolution of this contradiction is that l_{sl} starts to increase with L as $l_{sl} \approx L$ after reaching a minimum at $L = L_c$. It shall saturate, however when $L > l$ (in this case we are not bound to use Eq. 4 again ($L < l$!).

Eq.5 is not soluble analytically but assymptotics are easy to compute. For large l we get:

$$L_c/l = \exp(-\Theta_D/T), \tag{6}$$

which can be orders of magnitude small. When $l = 1$ we get $L_c = 1$.

The heat conductivity is proportional to l_{sl} (Eq.1) and should follow its behavior.

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